

Heat conduction in nanostructured polymers

Polymers are ubiquitous in our daily life, from biomolecules like DNA to plastics. Due to their unique properties, they can be found in a variety of applications, ranging from LED devices, to materials for aeronautics [1]. Yet, our understanding of how heat flows along polymer chains remains very incomplete, either at the single chain level or for bulk polymers having many chains in interaction [2]. Though a fundamental question, there is also an important challenge to enhance the intrinsic low thermal conductivity of polymers. This would open the way for their use in a wide range of applications, where heat dissipation is a critical issue, including microelectronics and packaging. Playing with the polymer morphology (see figures) is an as-yet unexplored way to change polymer heat conduction and it is the aim of the internship to study such a relation.

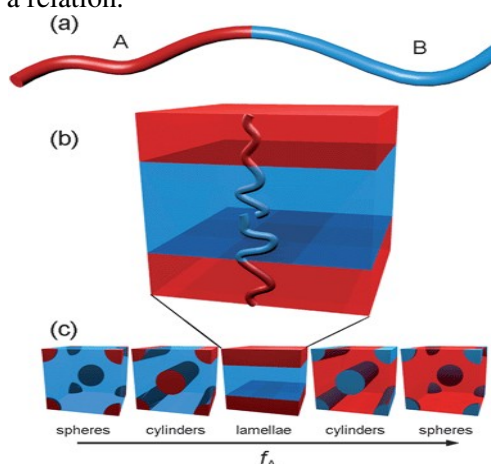
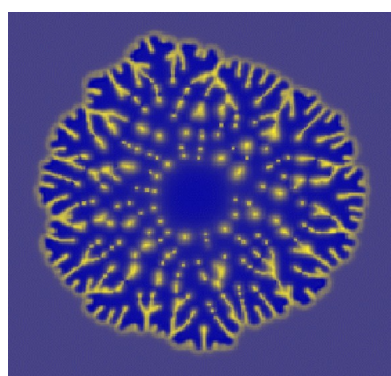


Figure: Polymer nanocrystallites (left, from [3]); block copolymer forming mesophases (right, from [4]).

To this end, the student will first run molecular dynamics simulations to probe heat flow in polymers, either at the single chain level or in heterogeneous polymers e.g. semi-crystalline or copolymers. Microscopic thermal transport properties will be next exploited in a mesoscopic code, with the aim of studying the interplay between heat flow and mesoscale structures. This internship is best suited for students having a taste for numerical simulations. No prior knowledge of polymer physics is required. The simulation results will be discussed in connection with experiments currently under way at the CETHIL (INSA Lyon) and at the IMP (UCBL).

Opening toward a PhD : yes (funding with «bourse ministère»)

- [1] H. Chen, V.V. Ginzburg, J. Yang, Y. Yang, W. Liu, Y. Huang, L. Du and B. Chen, « Thermal conductivity of polymer-based composites : fundamentals and applications », Prog. Poly. Sci. 59 (2016) 41-85
- [2] A. Henry, « Thermal transport in polymers », Annual Review in Heat Transfer, 17 (2013) 485-520
- [3] R. Laghmach, N. Candau, L. Chazeau, E. Munch and T. Biben, « Phase field modelling of strain induced crystal growth in an elastic matrix », J. Chem. Phys. 142 (2015) 244905
- [4] S. B. Darling, « Block copolymers for photovoltaics », Energy Env. Sci. 2 (2009) 1266-1273

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